

# GMBD Core Services

## Computational Proteomics

國立清華大學

生命科學系/生物資訊與結構生物研究所

# Introduction to protein structure analysis- tools, databases and the web resources: **ExPASy, Pfam, PDB**

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# ExPASy (**Expert Protein Analysis System**) proteomics server

**Switzerland:** <http://www.expasy.org/> at Swiss Institute of Bioinformatics, Geneva

**Australia:** <http://au.expasy.org/> at Australian Proteome Analysis Facility, Sydney

**Brazil:** <http://br.expasy.org/> at Laboratório Nacional de Computação Científica, Petrópolis

**Canada:** <http://ca.expasy.org/> at Canadian Bioinformatics Resource, Halifax

**Taiwan:** <http://tw.expasy.org/> at National Health Research Institute

**China:** <http://cn.expasy.org/> at Peking University

**Korea:** <http://kr.expasy.org/> at Yonsei Proteome Research Center, Seoul

# Introduction

- ExPASy是由瑞士生物資訊機構 ([Swiss Institute of Bioinformatics](#) , SIB) 所架設的伺服器。此伺服器包含了資料庫、工具&軟體、教育服務及一些相關連結。

Databases	Tools and software packages
<ul style="list-style-type: none"> <li>• <b>UniProt Knowledgebase (Swiss-Prot and TrEMBL)</b> - Protein knowledgebase</li> <li>• <b>ViralZone</b> - Portal to viral UniProtKB/Swiss-Prot entries</li> <li>• <b>PROSITE</b> - Protein families and domains</li> <li>• <b>SWISS-2DPAGE</b> - Two-dimensional polyacrylamide gel electrophoresis</li> <li>• <b>World-2DPAGE Repository</b> - A public standards-compliant repository for gel-based proteomics data published in the literature</li> <li>• <b>MIAPEGelDB</b> - A public repository for MIAPE Gel electrophoresis documents</li> <li>• <b>ENZYME</b> - Enzyme nomenclature</li> <li>• <b>GlycoSuiteDB</b> - a curated and annotated glycan database <small>new</small></li> <li>• <b>UniPathway</b> - Metabolic pathways</li> <li>• <b>SWISS-MODEL Repository</b> - Automatically generated protein models</li> </ul> <p>• Links to many other molecular biology databases</p>	<ul style="list-style-type: none"> <li>• <b>Proteomics and sequence analysis tools</b> <ul style="list-style-type: none"> <li>◦ Identification and characterization (Aldente, FindMod, Popitam, Phenyx, pl/Mw, ProtParam...)</li> <li>◦ DNA -&gt; Protein</li> <li>◦ Similarity searches (BLAST...)</li> <li>◦ Pattern and profile searches (ScanProsite...)</li> <li>◦ Post-translational modification and topology prediction</li> <li>◦ Primary structure analysis</li> <li>◦ Secondary and tertiary structure tools (Swiss-PdbViewer...)</li> <li>◦ Alignment and Phylogenetic analysis</li> </ul> </li> <li>• <b>Melanie / ImageMaster</b> - Software for 2-D PAGE analysis</li> <li>• <b>MSight</b> - Mass Spectrometry Imager</li> <li>• <b>Roche Applied Science's Biochemical Pathways</b></li> </ul>
Education and services	
<ul style="list-style-type: none"> <li>• <b>The ExPASy FTP server</b></li> <li>• <b>Swiss-Shop</b> - automatically obtain (by email) new sequence entries relevant to your field(s) of interest</li> <li>• Popular Science <ul style="list-style-type: none"> <li>◦ <b>Protein Spotlight</b></li> <li>◦ <b>Protéines à la «Une»</b></li> </ul> </li> <li>• <b>e-Proxemis</b> - Bioinformatics Learning Portal for Proteomics</li> </ul>	<ul style="list-style-type: none"> <li>• <b>Bioinformatics Core Facility for Proteomics</b></li> <li>• <b>Proteomics Core Facility</b> (formerly known as SWISS-2DSERVICE)</li> <li>• <b>SPS' Digest</b> - the Swiss Proteomics Society selection of proteomics articles</li> <li>• <b>Master's degree in Proteomics and Bioinformatics</b></li> <li>• <b>Swiss-Quiz</b></li> </ul>
Lists of molecular biology resources	
<ul style="list-style-type: none"> <li>• <b>ExPASy Life Science Directory</b> - The ExPASy list of biomolecular servers</li> <li>• <b>BioHunt</b> - Search the internet for molecular biology information</li> <li>• <b>The World-2DPAGE Constellation</b> - Promote and publish gel-based proteomics data through the ExPASy server</li> <li>• <b>WORLD-2DPAGE List</b> - Links to 2-D PAGE database servers and 2-D PAGE related servers and services</li> <li>• <b>World-2DPAGE Portal</b> - A dynamic portal to query simultaneously World-Wide gel-based proteomics databases</li> </ul>	
Swiss Institute of Bioinformatics (SIB) services	
<ul style="list-style-type: none"> <li>• <b>Vital-IT</b> - The HPC Center for Life Sciences</li> <li>• <b>Swiss node of EMBnet</b></li> <li>• <b>Ashbya Genome Database</b></li> <li>• <b>Cancer Immunome Database</b></li> </ul>	<ul style="list-style-type: none"> <li>• <b>CleanEx</b> - Gene expression database</li> <li>• <b>EPD</b> - Eukaryotic Promoter Database</li> <li>• <b>GermOnLine</b> - Knowledgebase on germ cell differentiation</li> <li>• <b>smRNAdb</b> - a database of small RNAs</li> <li>• <b>SwissRegulon</b> - a database of regulatory sites</li> </ul>

# Database

ExPASy所提供的資料庫包含了下列幾項：

## Databases

- **UniProt Knowledgebase (Swiss-Prot and TrEMBL)** - Protein knowledgebase
- **ViralZone** - Portal to viral UniProtKB/Swiss-Prot entries
- **PROSITE** - Protein families and domains
- **SWISS-2DPAGE** - Two-dimensional polyacrylamide gel electrophoresis
- **World-2DPAGE Repository** - A public standards-compliant repository for gel-based proteomics data published in the literature
- **MIAPEGeIDB** - A public repository for MIAPE Gel electrophoresis documents
- **ENZYME** - Enzyme nomenclature
- **GlycoSuiteDB** - a curated and annotated glycan database new
- **UniPathway** - Metabolic pathways
- **SWISS-MODEL Repository** - Automatically generated protein models
- [Links to many other molecular biology databases](#)

# UniProt Knowledgebase (Swiss-Prot and TrEMBL)

- ExPASy 本身是個資料庫的集合，主要所收集的資料是以蛋白質分子及蛋白質體組學為主的相關資料。其中 [UniProt Knowledgebase \(Swiss-Prot and TrEMBL\)](#) 是由SIB 和EBI (歐洲分子生物學機構)所共同維護的資料庫，也就是由Swiss-Prot、TrEMBL和PIR資料庫所聯合組成的Universal Protein Knowledgebase (UniProt)聯盟。主要包含了兩部分：



- ◆ **UniProtKB/Swiss-Prot:** 蛋白質序列資料庫，此資料庫提供高品質的注解 (annotation)，包含了蛋白質功能的描述、結構的描述、是否有後轉譯修飾(post-translational modifications)等。到2009年5月26日為止，共有468,851筆資料。



- ◆ **UniProtKB/TrEMBL:** TrEMBL可視為對Swiss-Prot的補充，利用電腦注解的方式補充Swiss-Prot的資訊。此資料包含了將所有EMBL核酸序列轉譯成蛋白質序列，並加註於可能的功能。到2009年5月26日為止，共有7,916,844筆資料。

**Notice:** This page will be replaced with [www.uniprot.org](http://www.uniprot.org). Please send us [your feedback!](#)

Search  for



**Swiss-Prot**  
**Protein knowledgebase**  
**TrEMBL**  
**Computer-annotated supplement to Swiss-Prot**

The [UniProt Knowledgebase](#) consists of:

- **UniProtKB/Swiss-Prot**; a curated protein sequence database which strives to provide a high level of annotation (such as the description of the function of a protein, its domains structure, post-translational modifications, variants, etc.), a minimal level of redundancy and high level of integration with other databases [[More details](#) / [References](#) / [Linking to Swiss-Prot](#) / [User manual](#) / [Recent changes](#) / [Disclaimer](#)].
- **UniProtKB/TrEMBL**; a computer-annotated supplement of Swiss-Prot that contains all the translations of EMBL nucleotide sequence entries not yet integrated in Swiss-Prot.

These databases are developed by the Swiss-Prot groups [at SIB](#) and [at EBI](#).

**UniProt Knowledgebase Release 15.3 consists of:**

**UniProtKB/Swiss-Prot Release 57.3 of 26-May-2009: 468851 entries** ([More statistics](#))

**UniProtKB/TrEMBL Release 40.3 of 26-May-2009: 0 entries** ([More statistics](#))

**> Swiss-Prot headlines**

Rotavirus: a serial killer in UniProtKB/Swiss-Prot ([Read more...](#))

### Access to the UniProt Knowledgebase

- [New UniProt web site](#) new
- [UniProtKB Taxonomy browser](#)
- [ViralZone](#) - Portal to viral UniProtKB/Swiss-Prot entries new
- [BLAST](#) similarity search
  
- [Retrieve a list of UniProtKB entries](#)
- [Randomly retrieve a UniProtKB entry](#)
- [UniProtKB Sequence/Annotation Version Database](#)
- [Swiss-Prot ID tracker](#)

<http://ca.expasy.org/sprot/>



# Prosite database

- PROSITE: Database of protein domains, families and functional sites.
- PROSITE 是由瑞士生物資訊研究所負責維護的資料庫，利用人工由文獻中蒐集資料整理而成。
- PROSITE 收集了在生物學上有顯著意義的蛋白質位點(site)和特定的序列模式(pattern)，並能根據這些位點(site)和模式(pattern)的資訊，利用電腦來進行快速鑑別工作，來鑑定一個未知功能的蛋白質序列應該屬於哪一個蛋白質家族以及可能的生物功能為何。





# Prosite database

## □ PROSITE patterns

- ◆ 一些具有生物重要性的胺基酸模式(**patterns**)。此模式可用 **regular expressions** 來表示。(e.g. [AC]-x-V-x(4)-{ED})。

## □ PROSITE profiles

- ◆ 有些蛋白質家族 (protein families)、生物功能或結構重要的區域(domains) 無法利用被 **PROSITE patterns** 所歸類出來，是因為這些蛋白質的序列是非常的 divergence，但可以利用 weight matrices (即 **profiles**) 的技術可以解決此一問題。
  - ◆ A profile is a table of position-specific amino acid weights and gap costs.
- Release 20.49, of 26-May-2009 (1555 documentation entries, 1308 patterns, 855 profiles and 861 ProRule)



## Database of protein domains, families and functional sites

**PROSITE** consists of [documentation entries](#) describing protein domains, families and functional sites as well as associated [patterns](#) and [profiles](#) to identify them [[More details](#) / [References](#) / [Disclaimer](#) / [Commercial users](#)].

PROSITE is complemented by **ProRule**, a collection of rules based on profiles and patterns, which increases the discriminatory power of profiles and patterns by providing additional information about functionally and/or structurally critical amino acids [[More details](#)].

**Release 20.49, of 26-May-2009 (1555 documentation entries, 1308 patterns, 855 profiles and 861 ProRule)**

### PROSITE access

e.g. PDOC00022, PS50089, SH3, zinc finger

 add wildcard '\*'

輸入AC或ID或pattern name  
Ex: hydrogenase or PS00747

Browse:

- [by documentation entry](#)
- [by ProRule description](#)
- [by taxonomic scope](#)
- [by number of positive hit](#)

### PROSITE tools

#### Scan a sequence

(Output includes graphical view and feature detection)



Enter your sequence or a UniProtKB (Swiss-Prot or TrEMBL) ID or AC [[help](#)]:

 exclude patterns with a high probability of occurrence

- [ScanProsite](#) - advanced scan

- [PRATT](#) - allows to interactively generate conserved patterns from a series of unaligned proteins.

- [MyDomains - Image Creator](#) <sup>new</sup> - allows to generate custom domain figures.



<http://ca.expasy.org/prosite/>

# Enzyme nomenclature database

- ENZYME是一個提供酵素命名相關搜尋的資料庫，而依據的**酵素命名方法**主要是由International Union of Biochemistry and Molecular Biology (IUBMB)提供，我們用此方法可以得到此酵素的EC (Enzyme Commission) number。

## 系統命名法：

1965年命名系統化，把所有酵素依催化反應分成六大類，以四組數字名之 (IUBMB 系統)；例如 histidine carboxylase 為 EC 4.1.1.22：

Main Class :	<u>4</u>	Lyases	分裂 C-C, C-O, C-N 鍵
Subclass :	<u>4.1</u>	C-C lyase	分裂 C-C 鍵
Sub-subclass :	<u>4.1.1</u>	Carboxylase	分裂 C-COO 鍵
序列號碼 :	<u>22</u>	第 22 個 4.1.1	分裂組胺酸的 C-COO 鍵

## IUBMB 系統所分的六個 Main Classes：

EC1	<u>Oxidoreductase</u>	氧化還原酶	電子或質子轉移
EC2	<u>Transferase</u>	轉移酶	官能基團的轉移
EC3	<u>Hydrolase</u>	水解酶	加水或脫水分子
EC4	<u>Lyase</u>	裂解酶	共價鍵生成或裂解
EC5	<u>Isomerase</u>	異構酶	同一分子內基團之轉移
EC6	<u>Ligase</u>	連接酶	消耗 ATP 生成分子間新鍵

# Access to ENZYME

- 直接輸入此酵素的**EC number**搜尋結果
- 用**Enzyme class**直接以酵素的分類方式找尋
- 輸入**Official name** 或是**Alternative name**搜尋結果
- 利用此酵素反應相關的**Chemical compound**搜尋
- 利用此酵素反應相關的**Cofactor**搜尋
- 用**Comments lines**來進行搜尋
- **SRS (Sequence Retrieval System)**

# Access to ENZYME

 [ExPASy Home page](#)

[Site Map](#)

[Search ExPASy](#)

[Contact us](#)

[PROSITE](#)

[Proteomics tools](#)

[Swiss-Prot](#)

Search  for



## ENZYME

### Enzyme nomenclature database

**ENZYME** is a repository of information relative to the nomenclature of enzymes. It is primarily based on the recommendations of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (IUBMB) and it describes each type of characterized enzyme for which an EC (Enzyme Commission) number has been provided [[More details](#) / [References](#) / [Linking to ENZYME](#) / [Disclaimer](#)].

**Release of 26-May-2009 (4141 active entries)**

#### Access to ENZYME

- by EC number:
- by enzyme class
- by description (official name) or alternative name(s):
- by chemical compound
- by cofactor
- by search in comments lines

輸入一組EC Number  
來搜尋結果

<http://ca.expasy.org/enzyme/>

# ExPASy

## Tools and software packages

ExPASy 蛋白質體工具

### Tools and software packages

- 
- **Proteomics and sequence analysis tools**
    - Identification and characterization (Aldente, FindMod, Popitam, Phenyx, pI/Mw, ProtParam...)
    - DNA -> Protein
    - Similarity searches (BLAST...)
    - Pattern and profile searches (ScanProsite...)
    - Post-translational modification and topology prediction
    - Primary structure analysis
    - Secondary and tertiary structure tools (Swiss-PdbViewer...)
    - Alignment and Phylogenetic analysis
  - **Melanie / ImageMaster** - Software for 2-D PAGE analysis
  - **MSight** - Mass Spectrometry Imager
  - **Roche Applied Science's Biochemical Pathways**

# Proteomics and sequence analysis tools

- 蛋白質身份辨識與理化特性分析 (Identification and characterization)
- 人工轉譯分析 (DNA -> Protein)
- 相似序列搜尋 (Similarity searches)
- 樣板序列搜尋與分析 (Pattern and profile searches)
- 轉譯後修飾預測 (Post-translational modification prediction)
- 拓樸特性預測分析 (Topology prediction)
- 一級結構分析 (Primary structure analysis)
- 二級結構分析 (Secondary structure prediction)
- 三級結構分析 (Tertiary structure)
- 序列比對 (Sequence alignment)
- 演化樹分析 (Phylogenetic analysis)
- 生物學關鍵字分析 (Biological text analysis)

# Pfam Database



[HOME](#) | [SEARCH](#) | [BROWSE](#) | [FTP](#) | [HELP](#)



## Pfam 23.0 (July 2008, 10340 families)

The Pfam database is a large collection of protein families, each represented by **multiple sequence alignments** and **hidden Markov models (HMMs)**. [More...](#)

### QUICK LINKS

- [SEQUENCE SEARCH](#)
- [VIEW A PFAM FAMILY](#)
- [VIEW A CLAN](#)
- [VIEW A SEQUENCE](#)
- [VIEW A STRUCTURE](#)
- [KEYWORD SEARCH](#)

### JUMP TO

### YOU CAN FIND DATA IN PFAM IN VARIOUS WAYS...

- Analyze your protein sequence for Pfam matches
- View Pfam family annotation and alignments
- See groups of related families
- Look at the domain organisation of a protein sequence
- Find the domains on a PDB structure
- Query Pfam by keywords

[Go](#) [Example](#)

Enter any type of accession or ID to jump to the page for a Pfam family or clan, UniProt sequence, PDB structure, etc.

Or view the [help](#) pages for more information

<http://pfam.sanger.ac.uk/>




# Databases for Protein Structure



# Molecular Biology Database Collection

~ more than 1000 databases

- [Nucleotide Sequence Databases](#)
- [RNA sequence databases](#)
- [Protein sequence databases](#)
- [Structure Databases](#) 
- [Genomics Databases \(non-vertebrate\)](#)
- [Metabolic and Signaling Pathways](#)
- [Human and other Vertebrate Genomes](#)
- [Human Genes and Diseases](#)
- [Microarray Data and other Gene Expression Databases](#)
- [Proteomics Resources](#)
- [Other Molecular Biology Databases](#)
- [Organelle databases](#)
- [Plant databases](#)
- [Immunological databases](#)

**The Molecular Biology Database Collection: 2008 update**  
Nucleic Acids Research, 2008, Vol. 36, Database issue **D2-D4**

- **Structure Databases**

- **Small molecules**

- [AANT - Amino Acid - Nucleotide interaction database](#)
    - [ChEBI - Chemical Entities of Biological Interest](#)
    - [ChemBank](#)
    - [ChemDB](#)
    - [CSD - Cambridge Structural Database](#)
    - [DrugBank](#)
    - [Het-PDB Navi](#)
    - [HIC-Up](#)
    - [Klotho](#)
    - [LIGAND](#)
    - [PDB-Ligand](#)
    - [PubChem](#)
    - [R.E.DD.B.](#)
    - [SuperDrug](#)
    - [SuperNatural](#)

- **Carbohydrates**

- [BCSDB/Glycoscience](#)
    - [CCSD - Complex Carbohydrate Structure Database \(CarbBank\)](#)
    - [CSS - Carbohydrate Structure Suite](#)
    - [Glycan](#)
    - [Glycoconjugate Data Bank](#)
    - [GlycoMapsDB](#)
    - [GlycoSuiteDB](#)
    - [Monosaccharide Browser](#)
    - [SWEET-DB](#)

- **Structure Databases**

- **Nucleic acid structure**

- [Greglist](#)
    - [GRSDB](#)
    - [ITS2](#)
    - [MeRNA](#)
    - [NCIR - Non-Canonical Interactions in RNA](#)
    - [NDB](#)
    - [NTDB](#)
    - [QuadBase](#)
    - [Rfam](#)
    - [RNA FRABASE](#)
    - [RNA SSTRAND](#)
    - [RNABase](#)
    - [RNAJunction](#)
    - [SARS-CoV RNA SSS](#)
    - [SCOR - Structural Classification Of RNA](#)
    - [Vir-Mir db](#)

- **Protein structure**

- [3D-Genomics](#)
    - [3DID - 3D interacting domains](#)
    - [ArchDB](#)
    - [ASTRAL](#)
    - [AutoPSI](#)
    - [BANMOKI](#)
    - [BioMagResBank](#)
    - [CADB - Conformational Angles DataBase of Proteins](#)
    - [CATH](#)
    - [CE](#)
    - [CoC Central](#)
    - [ColiSNP](#)

- Structure Databases

- Protein structure

- [Columba](#)
- [CSA - Catalytic Site Atlas](#)
- [Dali database](#)
- [DBAIi](#)
- [Decoys-R-U](#)
- [DisProt - Database of Protein Disorder](#)
- [DMAPS](#)
- [Dockground](#)
- [DomIns - Database of Domain Insertions](#)
- [DSDBASE - Disulfide Database](#)
- [DSMM - a Database of Simulated Molecular Motions](#)
- [E-MSD - EBI-Macromolecular Structure Database](#)
- [eF-site - Electrostatic surface of Functional site](#)
- [EzCatDB](#)
- [FireDB](#)
- [FSN](#)
- [Gene3D](#)
- [Genomic Threading Database](#)
- [GTOP - Genomes To Protein structures](#)
- [HOMSTRAD - Homologous Structure Alignment Database](#)
- [HotSprint](#)
- [IMB Jena Image Library](#)
- [IMGT/3Dstructure-DB](#)
- [IMOTdb](#)
- [MALISAM](#)
- [LPFC](#)
- [MegaMotifbase](#)
- [MMDB](#)
- [ModBase](#)
- [MolMovDB - Database of Macromolecular Movements](#)
- [PASS2](#)

- Structure Databases

- Protein structure

- [PDB](#)
- [PDB-REPRDB](#)
- [PDBselect](#)
- [PDBsum](#)
- [PDB\\_TM](#)
- [PepConfDB](#)
- [PFD - Protein Folding Database](#)
- [Phospho3D](#)
- [PIDD](#)
- [PMDB - Protein Model Database](#)
- [Structure Superposition Database](#)
- [ProSAS](#)
- [PROTCOM](#)
- [PRTAD](#)
- [RESID](#)
- [S4: Structure-based Sequence Alignments of SCOP Superfamilies](#)
- [SCOP - Structural Classification Of Proteins](#)
- [SCOPPI](#)
- [SitesBase](#)
- [SNAPPI](#)
- [SSToSS - Sequence-Structural Templates of Single-member Superfamilies](#)
- [STINGreport](#)
- [SUPERFAMILY](#)
- [SURFACE](#)
- [SWISS-MODEL Repository](#)
- [TargetDB](#)
- [TMBETA-GENOME](#)
- [TOPOFIT-DB](#)
- [TOPS - Topology Of Protein Structures](#)

# Protein Data Bank (PDB)

- <http://www.pdb.org/>
- Structure data determined by *X-ray crystallography* and *NMR*
- The data include the atom coordinate, reference, sequence, secondary structure, disulfide bond .....etc.

The number of protein structure and the last update date

MyPDB Login

A MEMBER OF THE PDB

An Information Portal to Biological Macromolecular Structures

As of Tuesday Jun 02, 2009 there are 57944 Structures | PDB Statistics

WHAT'S NEW | CONTACT | FEEDBACK | HELP | PRINT

PDB ID or keyword

Adv. Search

Home Search

- Home
- Getting Started
- Structural Genomics
- BioSync
- Electron Microscopy
- Download Files
- Deposit and Validate
- Dictionaries & File Formats
- Software Tools
- General Education
- General Information
- Acknowledgements
- Frequently Asked Questions

## A Resource for Studying Biological Macromolecules

The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the wwPDB, the RCSB PDB curates and annotates PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.

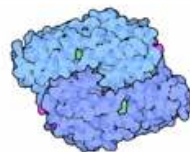
### Molecule of the Month: Vaults



Our cells are filled with compartments, each performing a specific function. Some of these compartments, such as mitochondria and lysosomes, are very large and enclose many different molecular machines. Other intracellular compartments are smaller, such as the transport vesicles that shuttle proteins from site to site inside the cell. Most of these compartments, including mitochondria, lysosomes and transport vesicles, are surrounded by membranes. However, in special cases, cells build smaller compartments surrounded by a protein shell. In our own cells, vaults are a spectacular example of these protein-enclosed compartments.

[Read more ...](#) [Previous Features](#)

### PSI Featured Molecule: Hda and DNA Replication



When cells divide, they need to ensure that each daughter cell gets one copy of each chromosome. Bacteria contain one big circle of DNA, so they start replication in one place, then copy the DNA both ways around until it finishes on the other side. PSI Researchers have solved the first atomic structure at how bacteria use the Hda protein to initiate replication at this origin only once for each generation of the cell.

[Read more from PSI SGKB](#) [Previous Features](#)

New user? Try the browser [compatibility check](#), information on [Getting Started](#), and see [What's New](#) on the site.

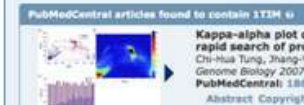
**PDB Statistics**  
**57944 Structures**  
**Last Update: Jun 02, 2009**

News

- Newsletter
- Discussion Forum
- Job Listings

02-June-2009

Literature View: Looking at Structures in PubMedCentral



The recently-released Literature View aims to provide a broad look at how a given structure has been analyzed and presented in open access publications, that is, where the full text of the article is available without copyright restriction. The overall intent is to make the PDB user more aware of publications associated with the structure under study.

[More >>](#)

### Data Snapshots

Time-stamped yearly snapshots of the PDB archive are available via FTP at: <ftp://snapshots.wwpdb.org> The snapshots provide readily identifiable data sets for research on the PDB archive.

## PDB Current Holdings Breakdown

	Proteins	Nucleic Acids	Protein/NA Complexes	Other	Total
X-ray	46383	1147	2141	17	49688
NMR	6864	856	146	6	7872
Exp. Method					
Electron Microscopy	168	16	59	0	243
Hybrid	13	1	1	1	16
Other	108	4	4	9	125
<b>Total</b>	<b>53536</b>	<b>2024</b>	<b>2351</b>	<b>33</b>	<b>57944</b>

(Click on any number to retrieve the results from that category.)

Please note that theoretical models have been removed, effective July 02, 2002, as per **PDB policy**.

**38858** structures in the PDB have a structure factor file.

**5156** structures in the PDB have an NMR restraint file.

- As Superfamilies Defined by SCOP
- As Superfamilies Defined by CATH

Use [Search Unreleased](#) to search and view entries that are currently being processed or are awaiting release.

Statistics are for experimentally-determined structures.

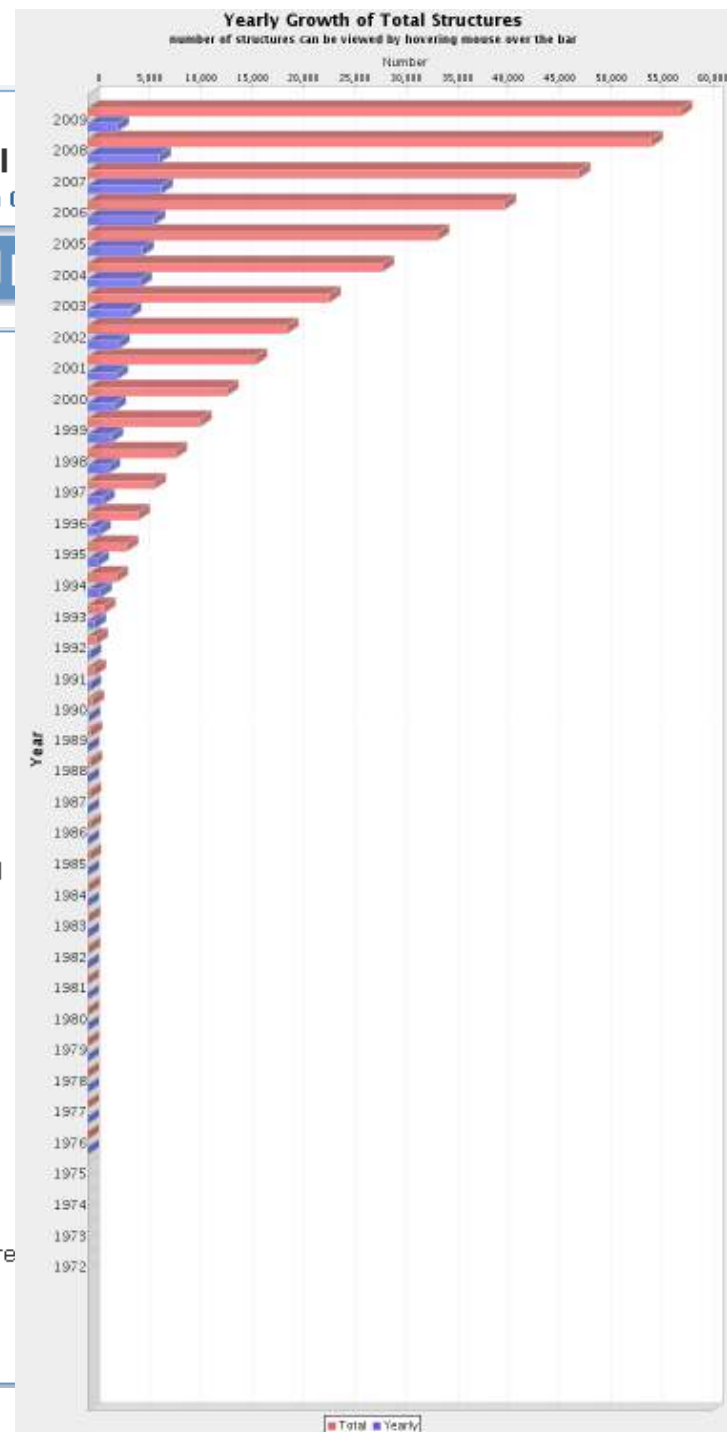


## PDB Statistics

- Content Distribution
  - [Summary Table of Released Entries](#)
  - [Status of Unreleased Entries](#)
  - [Proteins solved by multiple experimental methods](#)
  - [Redundancy based on sequence similarity](#)
  - [By Resolution](#)
  - [By Space Group](#)
  - [By Natural Source Organism](#)
  - [By Gene Source Scientific Organism](#)
  - [By Top 100 Journals](#)
  - [By Structural Genomics Centers](#)
  - [By Structure Molecular Weight](#)
  - [By Enzyme Classification](#)
- Content Growth
  - [Growth of Released Structures Per Year](#)
  - [Growth of Released Structures Per Year by Experimental Method](#)
    - [X-ray](#)
    - [NMR](#)
    - [Electron Microscopy](#)
  - [Growth of Released Structures Per Year by Molecular Type](#)
    - [Protein Only](#)
    - [DNA Only](#)
    - [RNA Only](#)
    - [Protein Nucleic Acid Complexes](#)
  - [Growth Of Unique Protein Classifications Per Year](#)
    - [As Folds Defined By SCOP](#)
    - [As Topologies Defined By CATH](#)
    - [As Superfamilies Defined By SCOP](#)
    - [As Superfamilies Defined By CATH](#)

Use [Search Unreleased](#) to search and view entries that are currently in the process of release.

Statistics are for experimentally-determined structures.





# Tutorial About This Site

*Flash*

**RCSB PDB**  
PROTEIN DATA BANK

WHAT'S NEW | CONTACT | FEEDBACK | HELP | PRINT

Home Search

- Home
- Getting Started**
- Structural Genomics
- BioSync
- Electron Microscopy
- Download Files
- Deposit and Validate
- Dictionaries & File Formats
- Software Tools
- General Education
- General Information
- Acknowledgements
- Frequently Asked Questions

## Getting Started

The RCSB PDB website provides

### Quick Start

*Navigation:* To navigate through the **General Education** section of the website, click on the **Getting Started** link in the left menu.

*Searching:* To search for structures, click on the **Search** link in the top navigation bar. For more detailed search options, see the **Search** page.

*Browsers and software:* **Most** of the structures are available in **Most** web browsers. A java-enabled browser and browser settings are required for some structures.

Some molecular viewers may require a **Flash** player.

## Website Organization

*Top Search Bar:* The top frame of the home page. Selecting the date will take you to the help desk.

*Left Menu:* Clicking on an arrow next to a link will take you to the help desk related to that topic. Clicking on a link will take you to the help desk related to that topic.

http://www.pdb.org/pdb/tutorials/Main\_Tutorial.swf - Windows Internet Explorer

http://www.pdb.org/pdb/tutorials/Main\_Tutorial.swf

http://www.pdb.org/pdb/tutorials/Main\_Tutorial.swf

Jump Menu

**Welcome to the RCSB PDB**

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their interactions to discover, function, and disease.

The RCSB is a member of the **wwPDB** whose mission is to ensure that the PDB archive contains an international resource with **uniform** data.

This Java site offers tools for browsing, searching, and reporting that allow the scientist and comprehensive data from the PDB community project.

Questions? [webmaster@rcsb.org](mailto:webmaster@rcsb.org)

Summary of Data in the Database

**Getting Started**

Please note that throughout the tutorial you may mouse over many options for a brief description and you can click on those options for longer text.

[http://www.pdb.org/pdb/tutorials/Main\\_Tutorial.swf](http://www.pdb.org/pdb/tutorials/Main_Tutorial.swf)

- Home
- Getting Started
- Structural Genomics
- BioSync
- Electron Microscopy
- Download Files
- Deposit and Validate
- Dictionaries & File Formats
- Software Tools
- General Education
- General Information
- Acknowledgements
- Frequently Asked Questions

## A Resource for Studying Macromolecules

The PDB archive contains information about proteins, nucleic acids, and complex assemblies. As a member of the PDB, you can search for PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of advanced searches based on annotations. Molecules are visualized, downloaded, and analyzed by specialized scientists.

**PDB ID or keyword**  
**Author**  
**Structural Genomics Center**  
**Chemical Name**  
**Chemical ID**

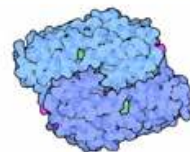
### Molecule of the Month: Vaults



Our cells are filled with compartments, each performing a specific function. Some of these compartments, such as mitochondria and lysosomes, are very large and enclose many different molecular machines. Other intracellular compartments are smaller, such as the transport vesicles that shuttle proteins from site to site inside the cell. Most of these compartments, including mitochondria, lysosomes and transport vesicles, are surrounded by membranes. However, in special cases, cells build smaller compartments surrounded by a protein shell. In our own cells, vaults are a spectacular example of these protein-enclosed compartments.

■ [Read more ...](#) ■ [Previous Features](#)

### PSI Featured Molecule: Hda and DNA Replication



When cells divide, they need to ensure that each daughter cell gets one copy of each chromosome. Bacteria contain one big circle of DNA, so they start replication in one place, then copy the DNA both ways around until it finishes on the other side. PSI Researchers have solved the first atomic structure at how bacteria use the Hda protein to initiate replication at this origin only once for each generation of the cell.

■ [Read more from PSI SGKB](#) ■ [Previous Features](#)

New user? Try the browser [compatibility check](#), information on [Getting Started](#), and see [What's New](#) on the site.

News  
Forum  
Looking at

Kappa-alpha plot de rapid search of prob  
Chi-Hua Tung, Zhang-Wu  
Genome Biology 2007, 8  
PubMedCentral: 13448  
Abstract Copyright

The recently-released Literature View aims to provide a broad look at how a given structure has been analyzed and presented in open access publications, that is, where the full text of the article is available without copyright restriction. The overall intent is to make the PDB user more aware of publications associated with the structure under study.

[More >>](#)

**Data Snapshots**

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# Advanced Search Interface

The screenshot displays the RCSB PDB Advanced Search Interface. At the top, the RCSB PDB logo is on the left, and navigation links like 'MyPDB Login' and 'A MEMBER OF THE PDB' are on the right. Below the logo, the text 'An Information Portal to Biological Macromolecular Structures' is centered, with a date and structure count below it. A search bar with a dropdown menu and a 'Search' button is present, with a red box and the number '1' highlighting the 'Adv. Search' button. On the left, a sidebar menu is visible, with the number '2' pointing to the 'Advanced Search' option. The main content area is titled 'Advanced Search Interface' and contains a 'Match all of the following conditions:' section. Below this, there are three rows of query type selection, each with an 'Evaluate Subquery' button. The number '3' is placed above the first 'Evaluate Subquery' button. A red arrow points to the '+' button next to the first 'Evaluate Subquery' button, with the text 'Add Query here!' written in red. The interface also features a list of query categories on the left, such as 'ID Search for Structures', 'Structural Genomics', 'Structure Summary', 'Ligand', and 'Biology & Chemistry'. On the right, there are more query categories like 'Expression Organism', 'Materials & Methods', and 'Primary Publication'. The bottom right corner shows the RCSB Protein Data Bank logo.

# Search PDB ID: 1L6H

The screenshot shows the RCSB PDB website interface. At the top left is the logo for RCSB PDB (Protein Data Bank). To the right, it says "A MEMBER OF THE wwPDB". Below this is the tagline "An Information Portal to Biological Macromolecular Structures" and a date/status line: "As of Tuesday Jun 02, 2009 there are 57944 Structures | PDB Statistics".

The search bar is located at the top center, with the text "PDB ID or keyword" and a dropdown menu showing "1l6h". To the right of the search bar is a "Search" button and a link to "Adv. Search".

On the left side, there is a navigation menu with links like "Home", "Getting Started", "Structural Genomics", "BioSync", "Electron Microscopy", "Download Files", "Deposit and Validate", "Dictionaries & File Formats", "Software Tools", "General Education", "General Information", "Acknowledgements", and "Frequently Asked Questions".

The main content area features a section titled "A Resource for Studying Biological Macromolecules". Below this is a paragraph describing the PDB archive and another paragraph about the tools and resources provided. There is a "Molecule of the Month: Vaults" section with a 3D model of a vault and a descriptive paragraph. At the bottom of the main content area, there is a note for new users: "New user? Try the browser compatibility check, information on Getting Started, and see What's New on the site."

On the right side, there is a "News" section with a "Click" button and a link to "Literature View: Looking at Structures in PubMedCentral". Below this is a "PubMedCentral articles found to contain 1FDM v" section with a small image and a link to "Kappa-alpha plot de rapid search of prot Chi-Hua Tung, Zhang-Wu Genome Biology 2007; PubMedCentral: 1868 Abstract Copyright".

Annotations on the page include red numbers 1, 2, and 3. Number 1 points to the search bar, number 2 points to the search results "1L6H" in a yellow box, and number 3 points to the "Click" button in the News section.

# Structure Summary : 1L6H

MSB **PDB** PROTEIN DATA BANK

An Information Portal to Biological Macromolecular Structures

As of Tuesday Jun 02, 2009 there are 57944 Structures | PDB Statistics

WHAT'S NEW | CONTACT | FEEDBACK | HELP | PRINT

PDB ID or keyword Search Adv. Search

Home Search Structures

- 1L6H
- Download Files
- FASTA Sequence
- Display Files
- Display Molecule
- Structural Reports
- External Links
- Structure Analysis
- Help
- Queries
- Reset View

Summary Derived Data Sequence Seq. Statistics Literature Biol. & Chem. Methods Geometry Lists

**Solution Structure of Plant nsLTP2 purified from Rice (oryza sativa)** **PDB ID** → **1L6H**

DOI:10.2210/pdb1l6h/pdb

Display Files \*  
Download Files \*  
Print this Page

**Primary Citation**

**Solution structure of plant nonspecific lipid transfer protein-2 from rice (Oryza sativa).**  
Samuel, D.,<sup>1</sup> Liu, Y.J.,<sup>1</sup> Cheng, C.S.,<sup>1</sup> Lys, P.C.<sup>1</sup>  
(2002) J.Biol.Chem. **277**: 35267-35272  
PubMed: 12011689 [ ] Search Related Articles in PubMed [ ]

Pubmed Abstract:  
The three-dimensional structure of rice nonspecific lipid transfer protein (nsLTP2) has been solved for the first time. The structure of nsLTP2 was obtained using 813 distance constraints, 30 hydrogen bond constraints, and 15 dihedral angle constraints. Fifteen of the 50 ... [ [Read More & Search PubMed Abstracts](#) ]

**Molecular Description** hide

Classification: **Lipid Transport** [ ]  
Structure Weight: 7017.06

Molecule: Non-Specific Lipid Transfer Protein  
Polymer: 1 Type: polypeptide(L) Length: 59  
Chain: A

**Source** hide

Polymer:	1	Scientific Name:	<b>Oryza sativa</b> [ ]	Common Name:	Rice
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**Derived Data** hide

- SCOP Classification v1.73 - (1 Domains)
- CATH Classification v3.2.0 - (1 Domains)
- PFAM Classification - (1 Domains)
- GO Terms - (3 Terms)

**Structure Image**



More Images...

3-D Viewers [ ]  
Jmol  
SimpleViewer  
Protein Workshop  
Other Viewers [ ]

**Deposition Summary** hide

Authors:	Samuel, D., <sup>1</sup> Liu, Y.J., <sup>1</sup> Cheng, C.S., <sup>1</sup> Lys, P.C. <sup>1</sup>
Deposit:	2002-03-11
Release:	2002-10-02
Last Modified (REVDAT):	2009-02-24

**Experimental Details** hide

Method: SOLUTION NMR  
Experimental Data: [ [BMRB](#) [ ] ]

**NMR Ensemble**

Conformers Calculated:	n/a
Conformers Submitted:	1
Selection Criteria:	N/A

**NMR Refine**

Method:	SOLUTION NMR
---------	--------------



# View Structure: 1L6H

The image displays a screenshot of the Protein Data Bank (PDB) website interface for structure 1L6H. The main content area is divided into several sections:

- Structure Image:** A red-bordered box highlights a ribbon diagram of the protein structure 1L6H, with the text "Structure Image" above it and "More Images..." below it.
- 3-D Viewers:** A section titled "3-D Viewers" lists several options: "Jmol", "SimpleViewer", "Protein Workshop", and "Other Viewers".
- Related Articles in PubMed:** A section titled "Related Articles in PubMed" shows a list of articles related to the structure, with a "hide" button.
- Structure Image:** A red-bordered box highlights a ribbon diagram of the protein structure 1L6H, with the text "Structure Image" above it and "More Images..." below it.

Overlaid on the website are four windows demonstrating different viewing methods:

- KiNG:** A window titled "KiNG" showing a ribbon diagram of the protein structure 1L6H. The window has a menu bar (File, Edit, Views, Display, Tools, Help) and a toolbar with options like "Pick center", "Show text", "Clipping", "Markers", and "Show hierarchy".
- Jmol:** A window titled "Jmol" showing a ribbon diagram of the protein structure 1L6H. The window has a menu bar (File, Edit, Views, Display, Tools, Help) and a toolbar with options like "Pick center", "Show text", "Clipping", "Markers", and "Show hierarchy".
- WebMol:** A window titled "WebMol" showing a ribbon diagram of the protein structure 1L6H. The window has a menu bar (File, Edit, Views, Display, Tools, Help) and a toolbar with options like "Pick center", "Show text", "Clipping", "Markers", and "Show hierarchy".
- Protein Workshop:** A window titled "Protein Workshop" showing a ribbon diagram of the protein structure 1L6H. The window has a menu bar (File, Edit, Views, Display, Tools, Help) and a toolbar with options like "Pick center", "Show text", "Clipping", "Markers", and "Show hierarchy".

The QuickPDB window shows a ribbon diagram of the protein structure 1L6H, with the text "QuickPDB" above it. The window has a menu bar (File, Edit, Views, Display, Tools, Help) and a toolbar with options like "Pick center", "Show text", "Clipping", "Markers", and "Show hierarchy".

# Sequence / Structure Details

Summary | Derived Data | **Sequence** | Seq. Similarity | Literature | Biol. & Chem. | Methods | Geometry | Links

Sequence / Structure Details **1L6H** [Display Files](#) [Download Files](#) [Print this Page](#)

**Redundancy Reduction and Sequence Clustering**  
View the **clustering results** for 1L6H.

**Sequence Display** ⓘ  
The structure **1L6H** has in total **1** chains. Out of these **1** are sequence-unique.  
Currently viewing **unique chains** only. [[show all chains](#)] [[show 3D in Jmol](#)]

**Chain Display**

Chain A (polymer 1) [[help](#)] [[fasta](#)] [[text/markup](#)]

Description: Non-Specific Lipid Transfer Protein  
Chain Type: polypeptide(L)  
**UniProt** reference: [Q10ST8](#)  
Length: 69 residues  
SCOP domain assignment: [d1l6ha](#) N on-specific lipid-transfer protein homologue (ns-LTP2): 69 residues ⓘ  
DSSP secondary structure: 46% helical (4 helices; 32 residues)  
More annotations:

Currently displayed: SEQRES sequence. [[display external \(UniProt/PIR\) sequence](#)]

Sequence Details

SCOP: **Non-specific lipid-transfer protein homologue (ns-LTP2) (d1l...**

DSSP:

PDB: **AGCNAGQLTVCTGAIAGGARPTAACCS SLRAQQGCFQCQFAKDPRYGRYVNSPNARKAVSS**

PDB: 1 10 20 30 40 50 60

SCOP: **Non-speci..**

DSSP:

PDB: **CGIALPTCH**

PDB: 61 69

# Biology and Chemistry Report

Summary | Derived Data | Sequence | Seq. Similarity | Literature | **Biol. & Chem.** | Methods | Geometry | Links

**Biology and Chemistry Report** **116h**

[Display Files ▼](#)  
[Download Files ▼](#)  
[Print this Page](#)

---

**Structure Details** ⓘ

**Structure Keywords**

Keywords	LIPID TRANSPORT
Text	naLTP2, Plant LTP, lipid transfer, LIPID TRANSPORT

**Polymeric Molecules**

**Chain A**

Description	Non-Specific Lipid Transfer Protein
Nonstandard Linkage	no
Nonstandard Monomers	no
Polymer Type	polypeptide(L)
Formula Weight	7017.1
Source Method	nat
Entity Name	LTP2

---

**Protein Details** ⓘ

**UniProt Information**

Chain	SWS/UNP ID	SWS/UNP Accession(s)
A	NLTPX_DRYSA	P83210 ⓘ

**Keywords and Names**

Chain(s)	RCSB Name	UNIPROT Name	UNIPROT Keywords
A	Non-Specific Lipid Transfer Protein	n/a	3D-structure , Direct protein sequencing , Disulfide bond , Lipid-binding , Signal , Transport

**GO Terms**

ⓘ Cellular Location | *F* Molecular Function | *P* Biological Process


**Chain A**

GO ID	Ontology	GO Term	Definition
6810 ⓘ	P	Transport	The Directed Movement of Substances (such As Macromolecules Small Molecules Ions) Into Out of Within or Between Cells or Within a Multicellular Organism.
6869 ⓘ	P	Lipid Transport	The Directed Movement of Lipids Into Out of Within or Between Cells. Lipids Are Compounds Soluble in an Organic Solvent But Not or Sparingly in an Aqueous Solvent.
8289 ⓘ	F	Lipid Binding	Interacting Selectively with a Lipid.



# Geometry

Summary | Derived Data | Sequence | Seq. Similarity | Literature | Biol. & Chem. | Methods | **Geometry** | Links

**Geometry**  **1I6h**

Structure Variance Analysis Results

Display Files ▾  
Download Files ▾  
Print this Page

RCSB Graphics

Chain Id | B factor | Omega | FDS Summary

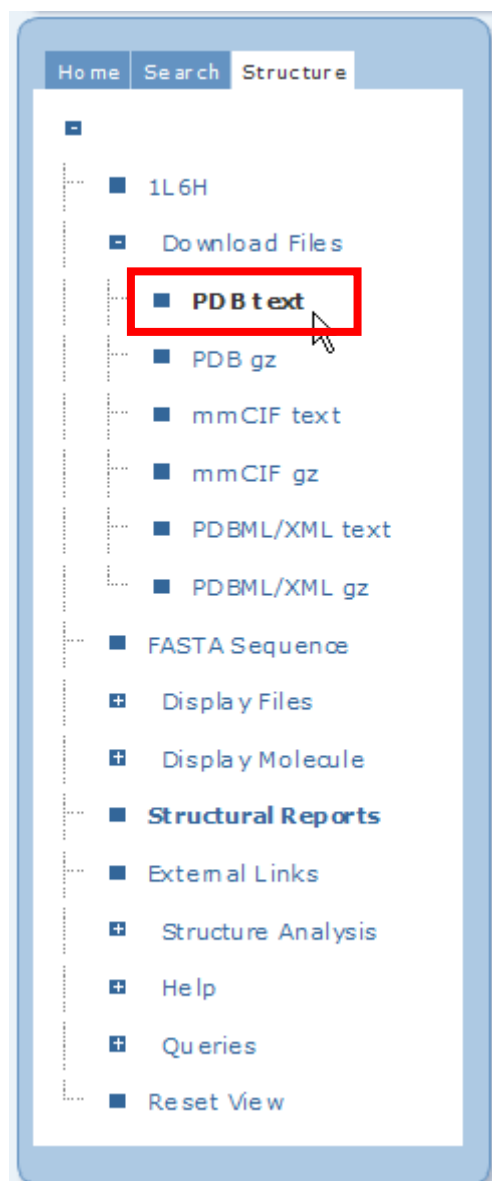
Dihedral Angle								
Dihedral Angle	Chain Id	Tot Num	Cal Ave	Cal StdDev	Std Val	Std StdDev	Minimum	Maximum
Chi1 g(+)	A	24	-69.88	14.272	-66.7	15.0	-113.10	-47.20
Chi1 g(-)	A	9	50.28	29.595	64.1	15.7	20.20	118.60
Chi1 trans	A	16	179.96	21.785	183.6	16.8	132.40	215.40
Omega	A	68	178.67	14.896	180	5.8	122.10	223.60
Phi	A	32	-39.37	91.899	-65.3	11.9	-163.50	164.00
Phi helix	A	32	-65.94	20.404	-65.3	11.9	-135.90	-32.70
Phi(P)	A	4	-71.53	4.447	-65.4	11.2	-78.50	-67.10
Psi	A	31	5.55	60.487	-39.4	11.3	-112.40	140.70
Psi helix	A	32	-31.66	20.700	-39.4	11.3	-75.90	28.00
Psi(G)	A	5	-25.90	75.476	-39.4	11.3	-154.60	61.30

Save Dihedral Angle Summary in:  CSV (Excel) Format  Save Report

N-CA-C(P)	A	4	111.79	2.223	111.8	2.5	108.98	115.21
N-CA-CB	A	36	109.55	2.926	110.5	1.7	102.16	117.49
N-CA-CB(A)	A	12	110.15	3.700	110.4	1.5	105.79	117.71
N-CA-CB(I,T,V)	A	9	107.27	2.518	111.5	1.7	102.25	110.77
N-CA-CB(P)	A	4	103.68	1.371	103.0	1.1	102.56	105.99
O-C-N	A	64	124.49	2.409	123.0	1.6	119.58	131.79
O-C-N(P)	A	4	124.59	0.675	122.0	1.4	123.85	125.30

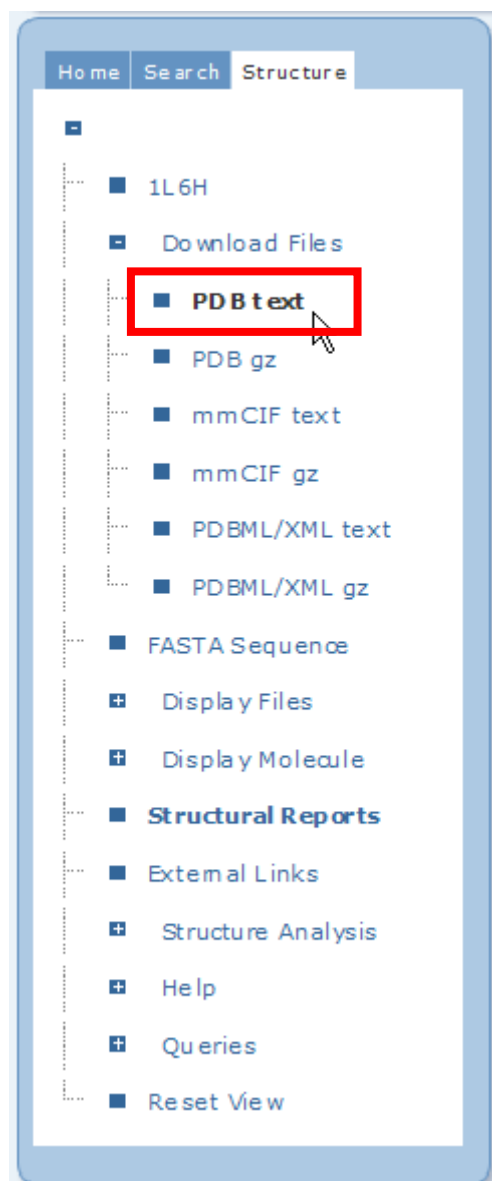
Save Bond Angle Summary in:  CSV (Excel) Format  Save Report

# Download/Display File



```
HEADER  LIPID TRANSPORT          11-MAR-02  1L6H
TITLE   SOLUTION STRUCTURE OF PLANT NSLTP2 PURIFIED FROM RICE
TITLE   2 (ORYZA SATIVA)
COMPND  MOL_ID: 1;
COMPND  2 MOLECULE: NON-SPECIFIC LIPID TRANSFER PROTEIN;
COMPND  3 CHAIN: A;
COMPND  4 SYNONYM: LTP2
SOURCE  MOL_ID: 1;
SOURCE  2 ORGANISM_SCIENTIFIC: ORYZA SATIVA;
SOURCE  3 ORGANISM_COMMON: RICE;
SOURCE  4 ORGANISM_TAXID: 4530
KEYWDS  NSLTP2, PLANT LTP, LIPID TRANSFER, LIPID TRANSPORT
EXPDTA  SOLUTION NMR
MDLTYP  MINIMIZED AVERAGE
AUTHOR  D.SAMUEL,P.-C.LYU
REVDAT  4 24-FEB-09 1L6H  1  VERSN
REVDAT  3 01-APR-03 1L6H  1  JRNL
REVDAT  2 04-FEB-03 1L6H  1  REMARK
REVDAT  1 02-OCT-02 1L6H  0
JRNL    AUTH  D.SAMUEL,Y.J.LIU,C.S.CHENG,P.C.LYU
JRNL    TTTL  SOLUTION STRUCTURE OF PLANT NONSPECIFIC LIPID
JRNL    TTTL 2 TRANSFER PROTEIN-2 FROM RICE (ORYZA SATIVA).
JRNL    REF   J.BIOL.CHEM.          V. 277 35267 2002
JRNL    REFN          ISSN 0021-9258
JRNL    PMID  12011089
JRNL    DOI   10.1074/JBC.M203113200
REMARK  1
REMARK  1 REFERENCE 1
REMARK  1 AUTH  Y.-J.LIU,D.SAMUEL,C.-H.LIN,P.-C.LYU
REMARK  1 TTTL  PURIFICATION AND CHARACTERIZATION OF A NOVEL 7-KDA
REMARK  1 TTTL 2 NON-SPECIFIC LIPID TRANSFER PROTEIN-2 FROM RICE
REMARK  1 TTTL 3 (ORYZA SATIVA)
REMARK  1 REF   BIOCHEM.BIOPHYS.RES.COMMUN. V. 294  535 2002
REMARK  1 REFN          ISSN 0006-291X
REMARK  1 DOI   10.1016/S0006-291X(02)00509-0
REMARK  2
REMARK  2 RESOLUTION. NOT APPLICABLE.
```

# Download/Display File



The screenshot shows the PDB website interface. At the top, there are navigation tabs: 'Home', 'Search', and 'Structure'. Below these is a sidebar menu with various options. The 'Download Files' section is expanded, and the 'PDB text' option is highlighted with a red box. Other options in the sidebar include '1L6H', 'PDB gz', 'mmCIF text', 'mmCIF gz', 'PDBML/XML text', 'PDBML/XML gz', 'FASTA Sequence', 'Display Files', 'Display Molecule', 'Structural Reports', 'External Links', 'Structure Analysis', 'Help', 'Queries', and 'Reset View'.

```
HELIX 1 1 GLN A 7 ALA A 16 1 10
HELIX 2 2 THR A 22 ALA A 40 1 19
HELIX 3 3 ARG A 44 VAL A 49 1 6
HELIX 4 4 ASN A 53 ALA A 57 5 5
SSBOND 1 CYS A 3 CYS A 35 1555 1555 2.02
SSBOND 2 CYS A 11 CYS A 25 1555 1555 2.04
SSBOND 3 CYS A 26 CYS A 61 1555 1555 2.04
SSBOND 4 CYS A 37 CYS A 68 1555 1555 2.05
CRYST1 1.000 1.000 1.000 90.00 90.00 90.00 P 1 1
ORIGX1 1.000000 0.000000 0.000000 0.000000
ORIGX2 0.000000 1.000000 0.000000 0.000000
ORIGX3 0.000000 0.000000 1.000000 0.000000
SCALE1 1.000000 0.000000 0.000000 0.000000
SCALE2 0.000000 1.000000 0.000000 0.000000
SCALE3 0.000000 0.000000 0.000000 0.000000
ATOM 1 N ALA A 1 42.576 -11.286 -3.123 1.00 0.00 N
ATOM 2 CA ALA A 1 42.743 -9.879 -3.389 1.00 0.00 C
ATOM 3 C ALA A 1 43.818 -9.551 -2.395 1.00 0.00 C
ATOM 4 O ALA A 1 43.756 -10.044 -1.336 1.00 0.00 O
ATOM 5 CB ALA A 1 41.585 -8.965 -2.979 1.00 0.00 C
ATOM 6 H1 ALA A 1 41.736 -11.706 -3.571 1.00 0.00 H
ATOM 7 H2 ALA A 1 42.601 -11.344 -2.083 1.00 0.00 H
ATOM 8 H3 ALA A 1 43.464 -11.717 -3.446 1.00 0.00 H
ATOM 9 HA ALA A 1 43.061 -9.768 -4.410 1.00 0.00 H
ATOM 10 HB1 ALA A 1 41.914 -7.920 -3.005 1.00 0.00 H
ATOM 11 HB2 ALA A 1 41.274 -9.133 -1.949 1.00 0.00 H
ATOM 12 HB3 ALA A 1 40.721 -9.055 -3.633 1.00 0.00 H
ATOM 13 N GLY A 2 44.716 -8.681 -2.942 1.00 0.00 N
ATOM 14 CA GLY A 2 45.682 -7.887 -2.232 1.00 0.00 C
ATOM 15 C GLY A 2 46.351 -8.666 -1.139 1.00 0.00 C
ATOM 16 O GLY A 2 46.368 -9.866 -1.120 1.00 0.00 O
ATOM 17 H GLY A 2 44.679 -8.358 -3.861 1.00 0.00 H
ATOM 18 HA2 GLY A 2 46.434 -7.585 -2.943 1.00 0.00 H
ATOM 19 HA3 GLY A 2 45.157 -7.003 -1.881 1.00 0.00 H
ATOM 20 N CYS A 3 46.781 -7.815 -0.201 1.00 0.00 N
```

# PDB File Title Section

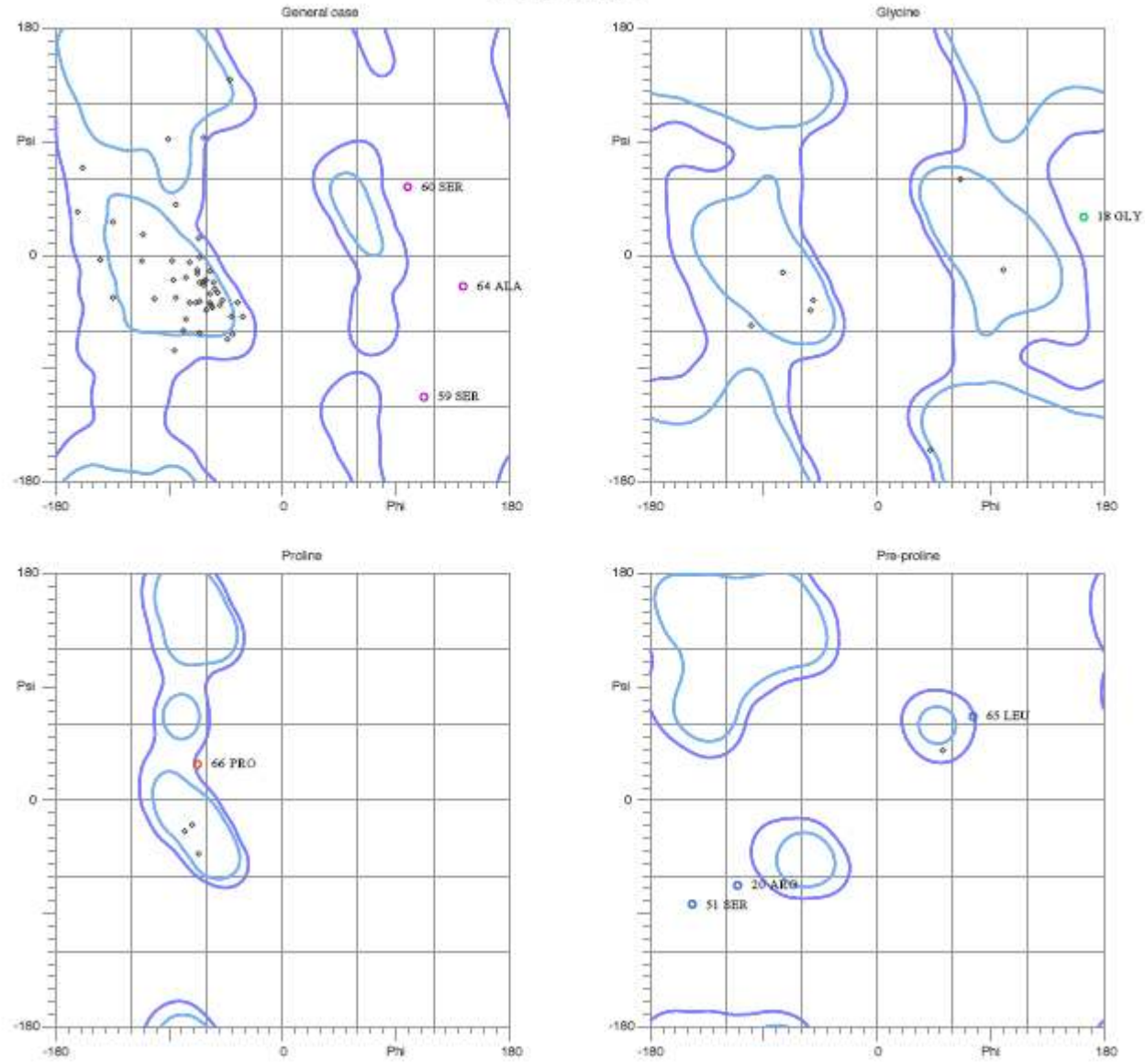
<b>HEAD</b>	First line of the entry, contains PDB ID code, classification, and date of deposition.	<b>HELIX</b>	Identification of helical substructures.
<b>COMPND</b>	Description of macromolecular contents of the entry.	<b>CRYST1</b>	Unit cell parameters, space group, and Z.
<b>SOURCE</b>	Biological source of macromolecules in the entry.	<b>ORIGXn</b>	Transformation from orthogonal coordinates to the submitted coordinates (n = 1, 2, or 3).
<b>AUTHOR</b>	List of contributors.	<b>SCALEn</b>	Transformation from orthogonal coordinates to fractional crystallographic coordinates (n = 1, 2, or 3).
<b>REVDAT</b>	Revision date and related information.	<b>MTRIXn</b>	Transformations expressing non-crystallographic symmetry (n = 1, 2, or 3). There may be multiple sets of these records.
<b>JRNL</b>	Literature citation that defines the coordinate set.	<b>ATOM</b>	Atomic coordinate records for standard groups.
<b>REMARK</b>	General remarks, some are structured and some are free form.	<b>HETATM</b>	Atomic coordinate records for heterogens.
<b>SEQRES</b>	Primary sequence of backbone residues.	<b>TER</b>	Chain terminator.
<b>FORMUL</b>	Chemical formula of non-standard groups.	<b>END</b>	Last record in the file.

# Ramachandran Plot

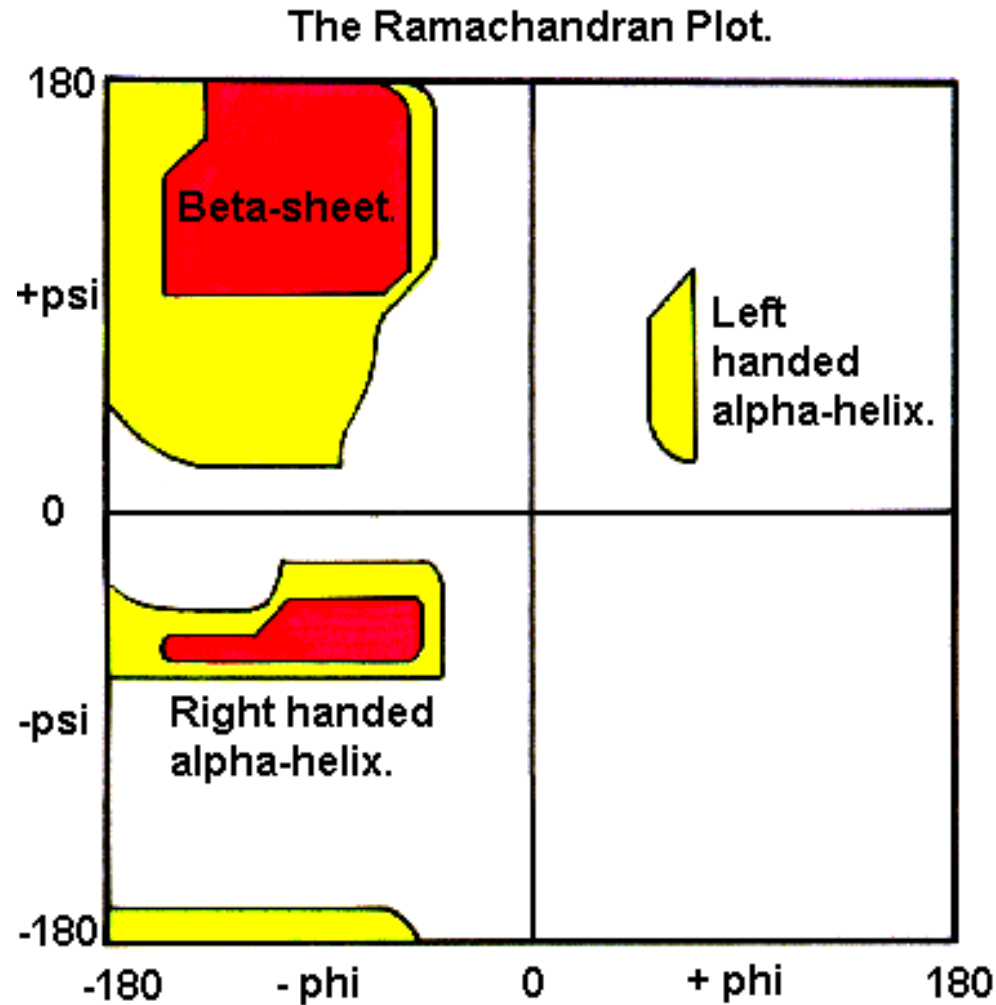
Home Search Structure

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    - PDB gz
    - mmCIF text
    - mmCIF gz
    - PDBML/XML text
    - PDBML/XML gz
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      - RCSB Tables
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1L6H, model 1



# Ramachandran plot



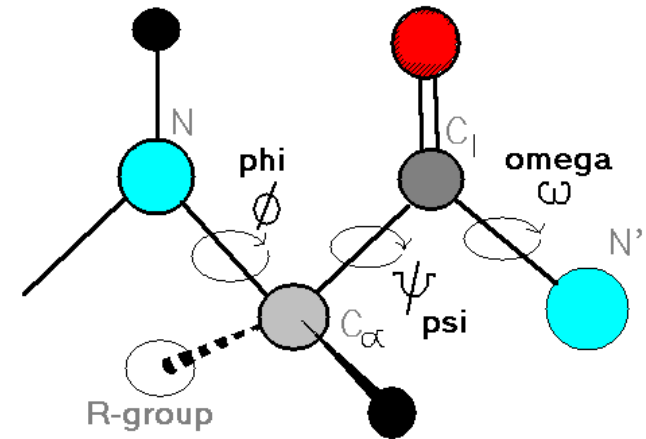
## $\beta$ -strand:

$$-180 < \phi < -60$$

$$180 > \psi > 60$$

## $\alpha$ -helix:

$$\phi: \sim -60$$



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## BIOLOGICAL DETAILS

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- [GeneCensus](#)
- [IEDB](#) : *No external link available*
- [CSA](#) : *No external link available*

## EXPERIMENTAL DATA

- [Electron Microscopy Database \(EMDB\)](#) : *No external link available*
- [Electron Density Server \(EDS\)](#)

## GEOMETRY

- [WHAT\\_CHECK \(WHAT IF\)](#)
- [PROCHECK](#)

## PATHWAYS

- [METACYC](#) : *No external link available*

## PROTEIN MOTIONS

- [Molecular Movements Database \(MMD\)](#)

# External Links

## SECONDARY STRUCTURE

- [Secondary Structure Assignments \(DSSP\)](#)

## STRUCTURE CLASSIFICATION

- [DALI](#)
- [Flexible structure Alignment by Chaining Aligned fragment pairs allowing Twists \(FATCAT\)](#)
- [Structural Classification of Proteins \(SCOP\)](#)
- [Protein Structure Classification \(CATH\)](#)
- [Vector Alignment Search Tool \(VAST\)](#)

## STRUCTURE FEATURES

- [Computed Atlas of Surface Topography of proteins \(CASTp\)](#)
- [Gaussian Network Model \(GNM\)](#)
- [Analysis of interatomic Contacts of Structural Units \(CSU\)](#)
- [Analysis of Ligand-Protein Contacts \(LPC\)](#)
- [SWISS-MODEL](#) : *No external link available*
- [Homology derived Secondary Structure of Proteins \(HSSP\)](#)

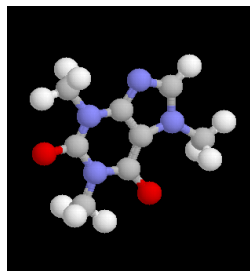
## STRUCTURE SUMMARY

- [Molecular Modeling DataBase \(NCBI/Entrez\) \(MMDB\)](#)
- [OCA Browser \(OCA\)](#)
- [Protein Data Bank Japan \(wwPDB Partner\) \(PDBj\)](#)
- [Protein Quaternary Structure \(PQS\)](#)
- [Proteopedia](#)
- [Biological Magnetic Resonance Data Bank \(BMRB\)](#)
- [Protein Databank in Europe \(PDBe\)](#)
- [PDBsum](#)
- [Jena Library](#)

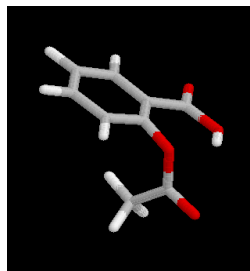


# Molecular Graphics

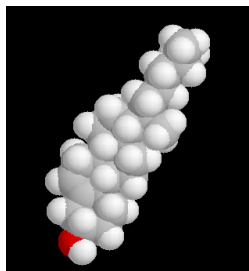
- 是一種可顯現出生物巨分子結構的軟體，包含蛋白質、**DNA**、**RNA**、化學小分子和金屬等皆可藉由視覺化軟體來呈現他們的結構。
- 視覺化的軟體可以輔助觀察巨分子的結構、作用力、表面特性等。尤其在藥物設計、分子模擬上有很大的應用空間。



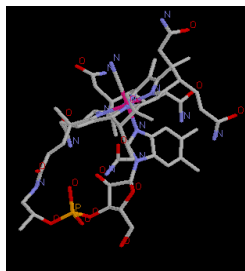
咖啡因



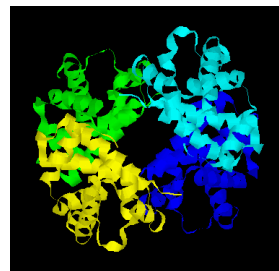
阿斯匹靈



膽固醇



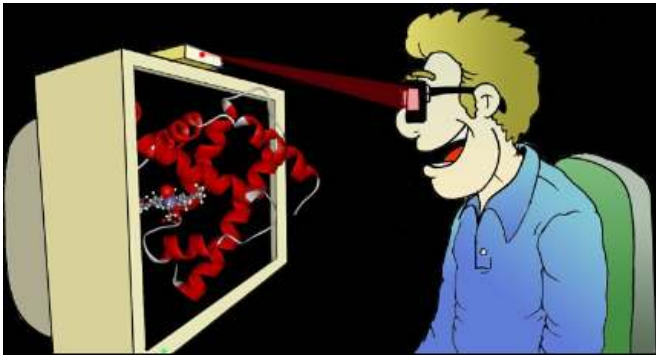
維生素B<sub>12</sub>



血紅蛋白

# Molecular Graphics

- MDL Chime
- RasMol
- PyMOL
- Cn3D
- Swiss PDB viewer
- MOLMOL
- MolScript
- Raster3D
- GRASP
- WebLabViewer



**Thank you!**